

Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 05:33 PM EDT

PDB ID : 4Z8F

Title: Fab structure of antibody S1-15 in complex with ssDNA DNA, 5'-p5(dT)p-3'

Authors: Haji-Ghassemi, O.; Evans, S.V.

Deposited on : 2015-04-08

Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

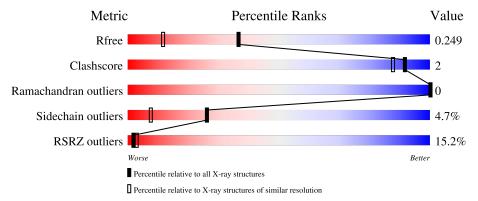
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range}(\mathring{\rm A})) \end{array}$		
R_{free}	130704	2340 (1.76-1.76)		
Clashscore	141614	2466 (1.76-1.76)		
Ramachandran outliers	138981	2437 (1.76-1.76)		
Sidechain outliers	138945	2437 (1.76-1.76)		
RSRZ outliers	127900	2298 (1.76-1.76)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain					
1	Н	227	17%	93%		7%			
2	L	214	12%	93%		7%			
3	A	5	20%						
3	Е	5		60%	20%	20%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called S1-15 Fab (IgG2b) heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	П	226	Total	С	N	О	S	0	0	0
1	11	220	1710	1080	284	336	10	0	0	

• Molecule 2 is a protein called S1-15 Fab (IgG2b kappa) light chain.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	L	214	Total 1668	C 1032	N 283	O 345	S 8	0	1	0

• Molecule 3 is a DNA chain called 5'-D(P*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
2	E	4	Total	С	N	О	Р	0	0	0
) E	4	65	30	6	25	4	U	U		
9	3 A	9	Total	С	N	О	Р	0	0	1
3		3	45	20	4	18	3	U		1

• Molecule 4 is water.

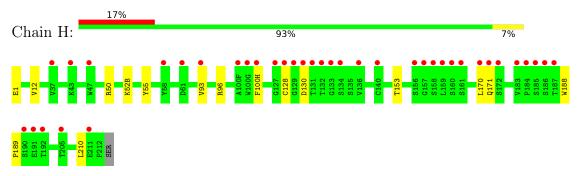
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	86	Total O 86 86	0	0
4	L	101	Total O 101 101	0	0
4	Е	7	Total O 7 7	0	0
4	A	2	Total O 2 2	0	0



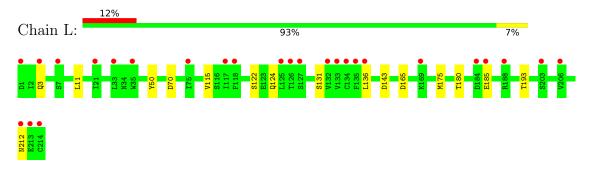
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: S1-15 Fab (IgG2b) heavy chain



• Molecule 2: S1-15 Fab (IgG2b kappa) light chain

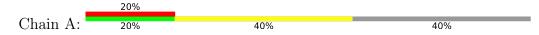


• Molecule 3: 5'-D(P*TP*TP*TP*TP*T)-3'





• Molecule 3: 5'-D(P*TP*TP*TP*TP*T)-3'







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	77.58Å 77.58Å 156.27Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 - 1.75	Depositor
rtesolution (A)	24.69 - 1.75	EDS
% Data completeness	99.7 (25.00-1.75)	Depositor
(in resolution range)	99.8 (24.69-1.75)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	4.33 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.80073	Depositor
P. P.	0.208 , 0.240	Depositor
R, R_{free}	0.217 , 0.249	DCC
R_{free} test set	2438 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 40.8	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3684	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: THP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	nd lengths	Bond	angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	Н	0.50	0/1756	0.65	0/2398
2	L	0.50	0/1704	0.67	0/2311
3	A	2.07	1/22~(4.5%)	0.67	0/33
3	Е	1.12	$1/70 \ (1.4\%)$	0.65	0/105
All	All	0.54	$2/3552 \ (0.1\%)$	0.66	0/4847

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	A	6	DT	O3'-P	-9.62	1.49	1.61
3	Е	10	DT	OP3-P	-8.99	1.50	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Н	1710	0	1653	6	0
2	L	1668	0	1596	5	0
3	A	45	0	24	0	0
3	Ε	65	0	36	1	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Е	7	0	0	0	0
4	Н	86	0	0	1	0
4	L	101	0	0	2	0
All	All	3684	0	3309	11	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
2:L:165:ASP:HB2	4:L:377:HOH:O	1.70	0.92
2:L:131:SER:OG	2:L:180:THR:HG22	1.87	0.74
1:H:50:ARG:NH1	3:E:10:DT:OP3	2.39	0.55
2:L:180:THR:HG23	4:L:376:HOH:O	2.08	0.53
1:H:93:VAL:HG11	1:H:100(H):PHE:HB3	1.92	0.51
1:H:93:VAL:CG1	1:H:100(H):PHE:HB3	2.41	0.50
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.76	0.49
1:H:52(B):LYS:HD3	1:H:55:TYR:CE2	2.49	0.47
2:L:115:VAL:HG22	2:L:136:LEU:HD22	1.98	0.44
1:H:188:TRP:CG	1:H:189:PRO:HA	2.54	0.43
1:H:1:GLU:HG3	4:H:370:HOH:O	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	Н	$224/227 \ (99\%)$	223 (100%)	1 (0%)	0	100	100
2	L	$212/214 \ (99\%)$	209 (99%)	3 (1%)	0	100	100
All	All	436/441 (99%)	432 (99%)	4 (1%)	0	100	100



There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	Н	190/191 (100%)	182 (96%)	8 (4%)	30	9	
2	L	193/192 (100%)	183 (95%)	10 (5%)	23	6	
All	All	383/383 (100%)	365 (95%)	18 (5%)	26	7	

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	12	VAL
1	Н	96	ARG
1	Н	128	CYS
1	Н	130	ASP
1	Н	153	THR
1	Н	170	LEU
1	Н	171	GLN
1	Н	210	LEU
2	L	3	GLN
2	L	11	LEU
2	L	50	TYR
2	L	70	ASP
2	L	122	SER
2	L	143	ASP
2	L	175	MET
2	L	185	GLU
2	L	193	THR
2	L	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	124	GLN
2	L	212	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	THP	A	8	3	23,25,26	0.59	0	31,37,40	0.74	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THP	A	8	3	-	4/12/26/27	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
3	A	8	THP	C2'-C1'-N1	2.31	119.08	113.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	8	THP	C2'-C1'-N1-C6
3	A	8	THP	C2'-C1'-N1-C2
3	A	8	THP	O4'-C1'-N1-C6
3	A	8	THP	O4'-C1'-N1-C2



There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	Н	$226/227 \ (99\%)$	0.89	38 (16%) 1 2	23, 35, 85, 98	0
2	L	214/214 (100%)	0.66	26 (12%) 4 6	23, 37, 57, 79	0
3	A	2/5~(40%)	3.49	1 (50%) 0 0	45, 45, 45, 62	0
3	Е	4/5 (80%)	2.04	3 (75%) 0 0	46, 53, 56, 65	0
All	All	446/451 (98%)	0.80	68 (15%) 2 3	23, 37, 75, 98	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	214[A]	CYS	8.9
1	Н	132	THR	8.7
1	Н	128	CYS	7.7
1	Н	157	GLY	7.5
1	Н	129	GLY	6.6
1	Н	187	THR	6.0
1	Н	131	THR	6.0
1	Н	133	GLY	5.8
1	Н	134	SER	5.8
1	Н	159	LEU	5.7
1	Н	156	SER	5.7
1	Н	130	ASP	5.4
3	A	6	DT	5.4
1	Н	160	SER	4.4
1	Н	185	SER	4.1
1	Н	158	SER	4.1
2	L	133	VAL	4.0
2	L	135	PHE	4.0
2	L	206	VAL	3.9
1	Н	127	GLY	3.9
1	Н	161	SER	3.8

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Mol	Chain	$\frac{i \ previous}{\mathbf{Res}}$	Type	RSRZ
1	Н	183	VAL	3.7
1	Н	172	SER	3.5
1	Н	140	CYS	3.3
1	Н	136	VAL	3.3
1	Н	191	GLU	3.3
1	Н	186	SER	3.2
2	L	212	ASN	3.1
1	Н	171	GLN	3.1
1	Н	61	ASP	3.1
1	Н	170	LEU	3.0
1	Н	93	VAL	2.9
2	L	125	LEU	2.9
1	Н	184	PRO	2.9
2	L	35	TRP	2.8
2	L	132	VAL	2.8
2	L	188	ARG	2.8
2	L	117	ILE	2.7
2	L	134	CYS	2.7
1	Н	100(G)	TRP	2.7
1	Н	37	VAL	2.7
1	Н	211	GLU	2.6
2	L	127	SER	2.6
3	Ε	10	DT	2.6
2	L	75	ILE	2.6
2	L	3	GLN	2.6
2	L	1	ASP	2.5
1	Н	190	SER	2.5
2	L	126	THR	2.5
2	L	136	LEU	2.5
2	L	118	PHE	2.5
1	Н	58	TYR	2.4
2	L	184	ASP	2.4
2	L	213	GLU	2.4
1	Н	100(H)	PHE	2.3
3	Е	11	DT	2.3
2	L	33	LEU	2.3
2	L	21	ILE	2.3
1	Н	100(F)	ALA	2.3
2	L	7	SER	2.2
1	Н	205	THR	2.2
3	Е	12	DT	2.2
1	Н	43	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	169	LYS	2.1
1	Н	192	THR	2.1
2	L	185	GLU	2.1
1	Н	47	TRP	2.1
2	L	203	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	THP	A	8	24/25	0.94	0.12	28,34,41,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

